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DESY.

KISS

CaloHadronic : a diffusion model for the generation of hadronic showers

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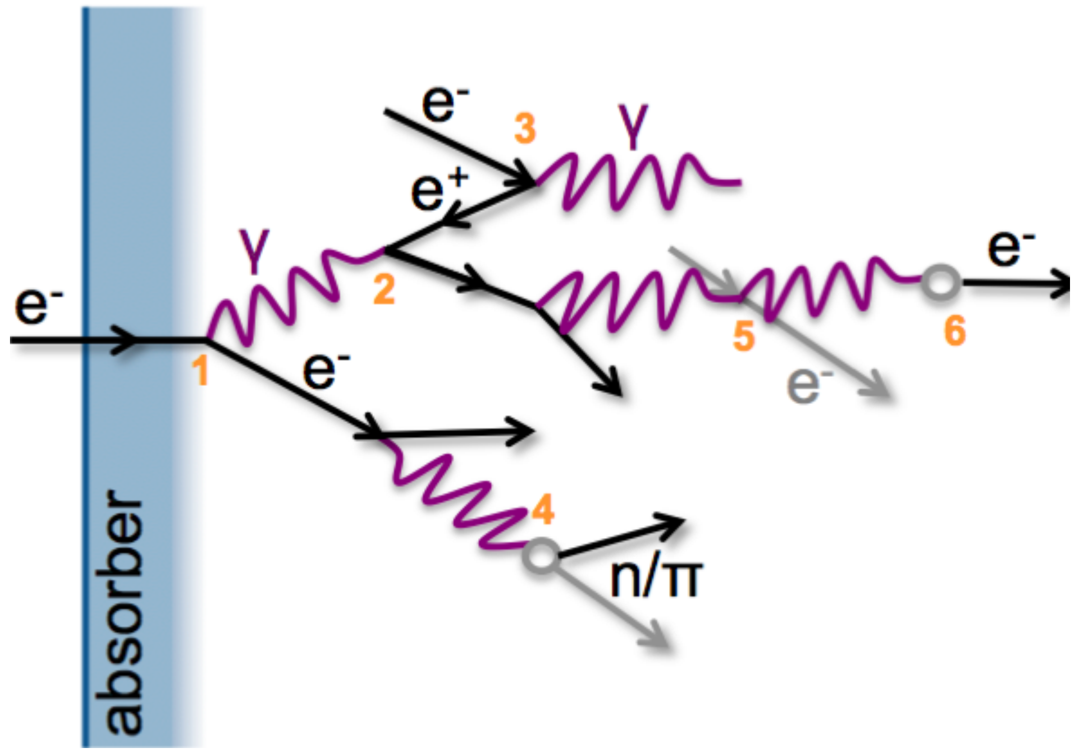
Generative model for em and hadronic showers

CaloClouds II [1] ⟶ Fast & accurate point clouds based generative model applied **only to electromagnetic showers**

[1] **CaloClouds II: Ultra-Fast Geometry-Independent Highly-Granular Calorimeter Simulation**
E. Buhmann et al: arxiv: 2309.05704



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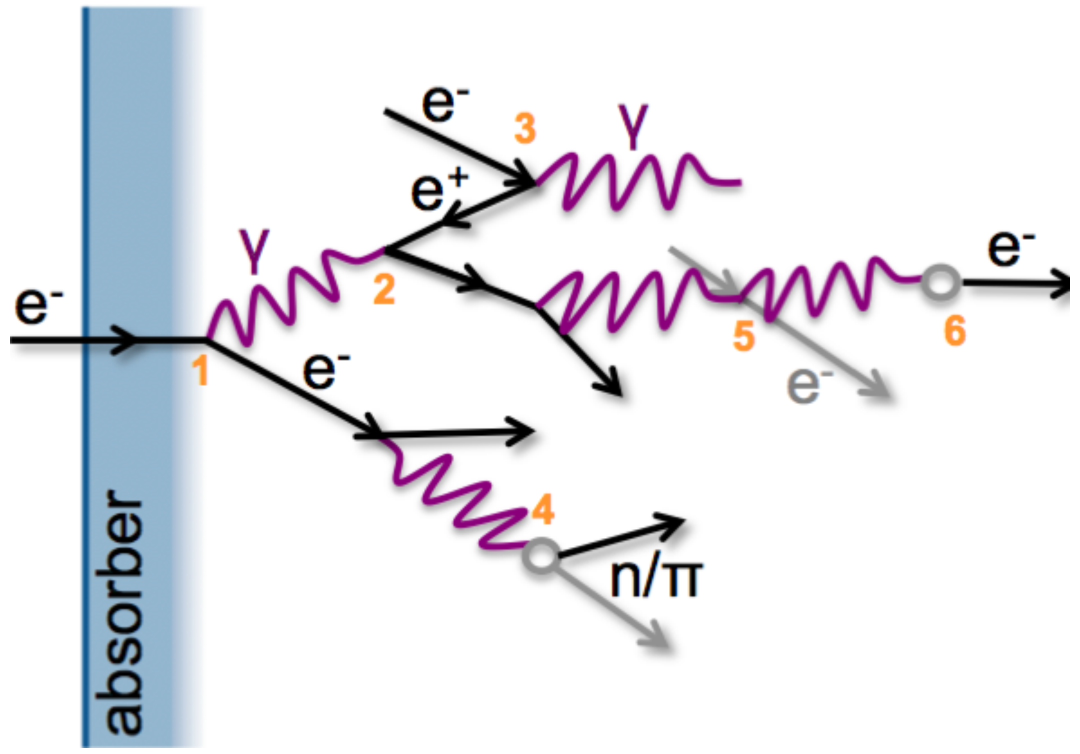


Now

↓

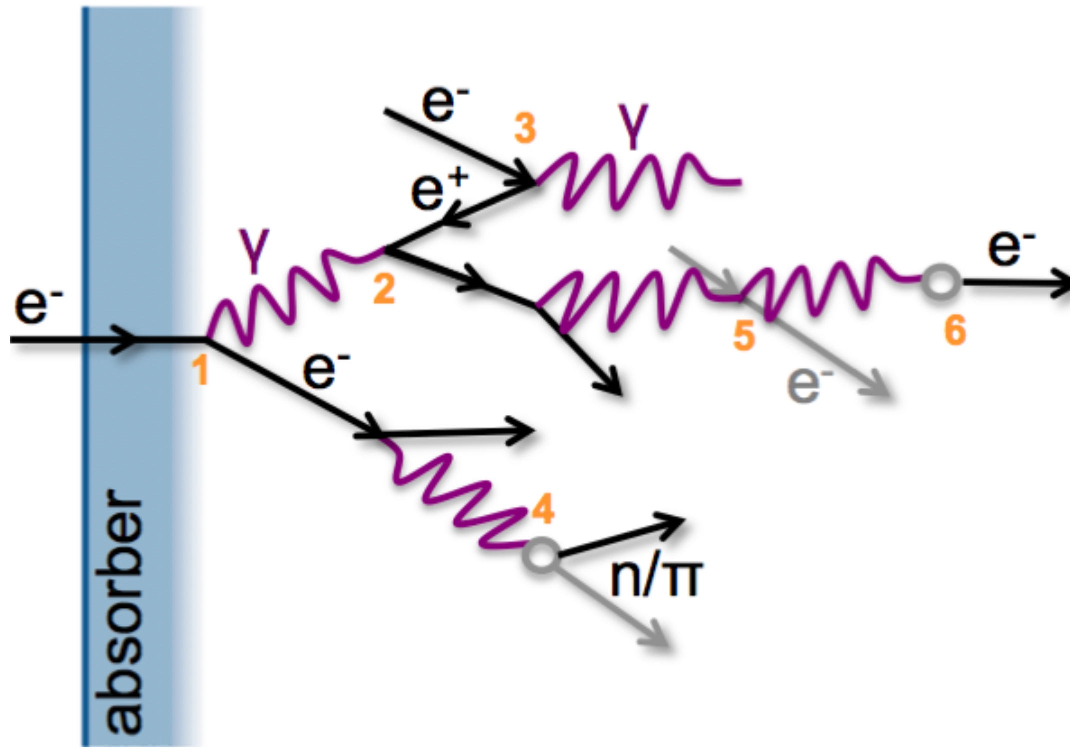
HADRONIC showers

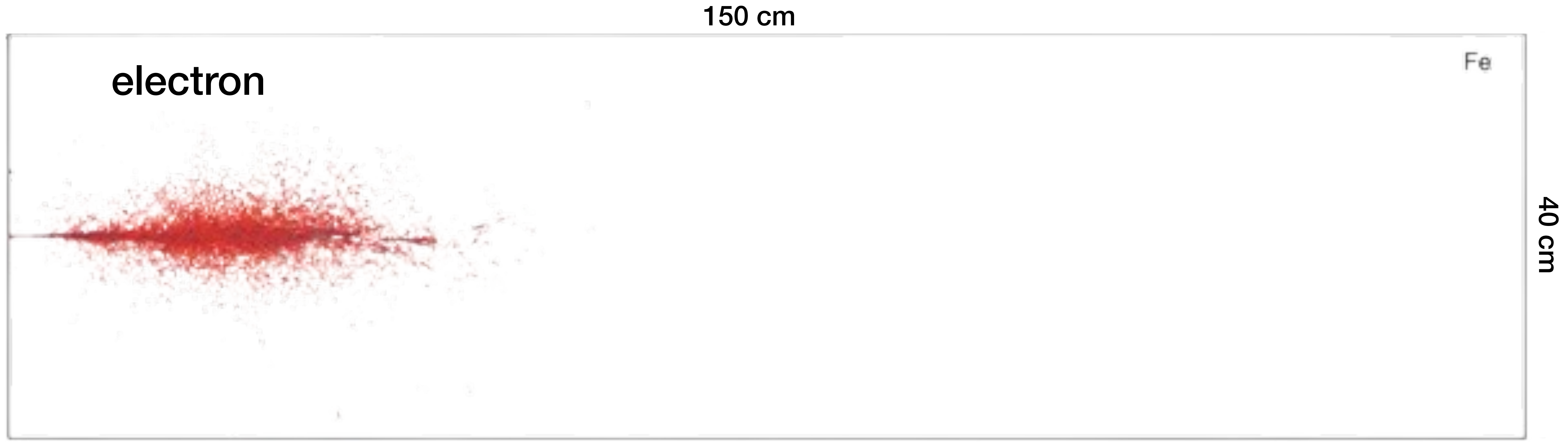
Dealing with 10-90 GeV π^+ showers
two components: hadronic and electromagnetic

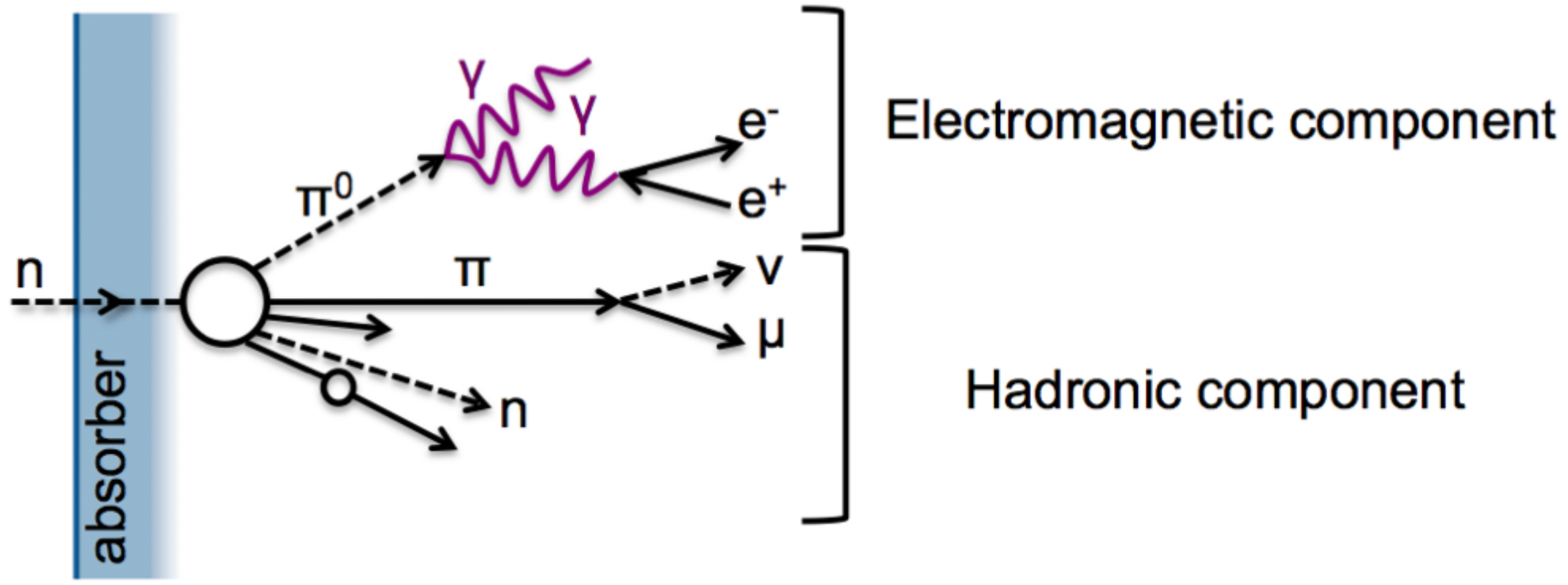
Hadron showers have **much larger:**

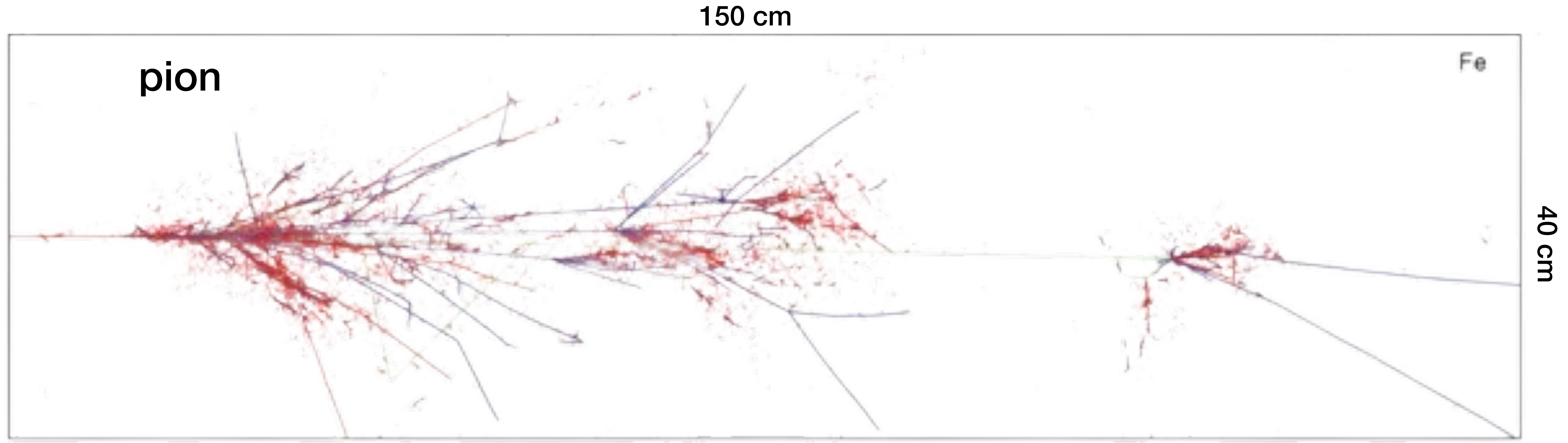
- **spatial extension** -> interaction length larger than radiation length
- **lateral dispersion** -> large transverse energy transfers in nuclear reactions

Em and hadronic showers









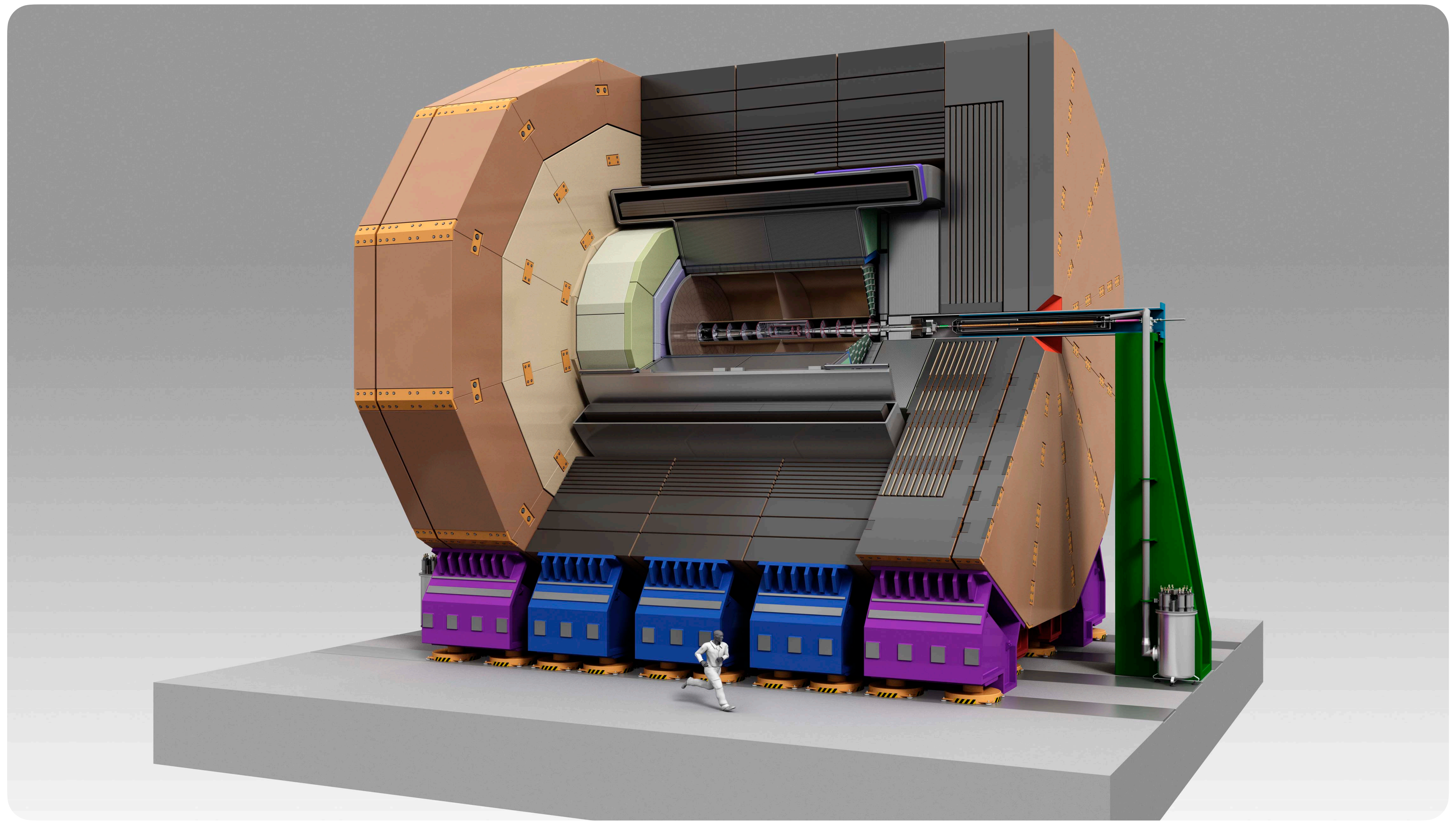
Hadronic cascades are much more complex than em cascades!

ILD calorimeter

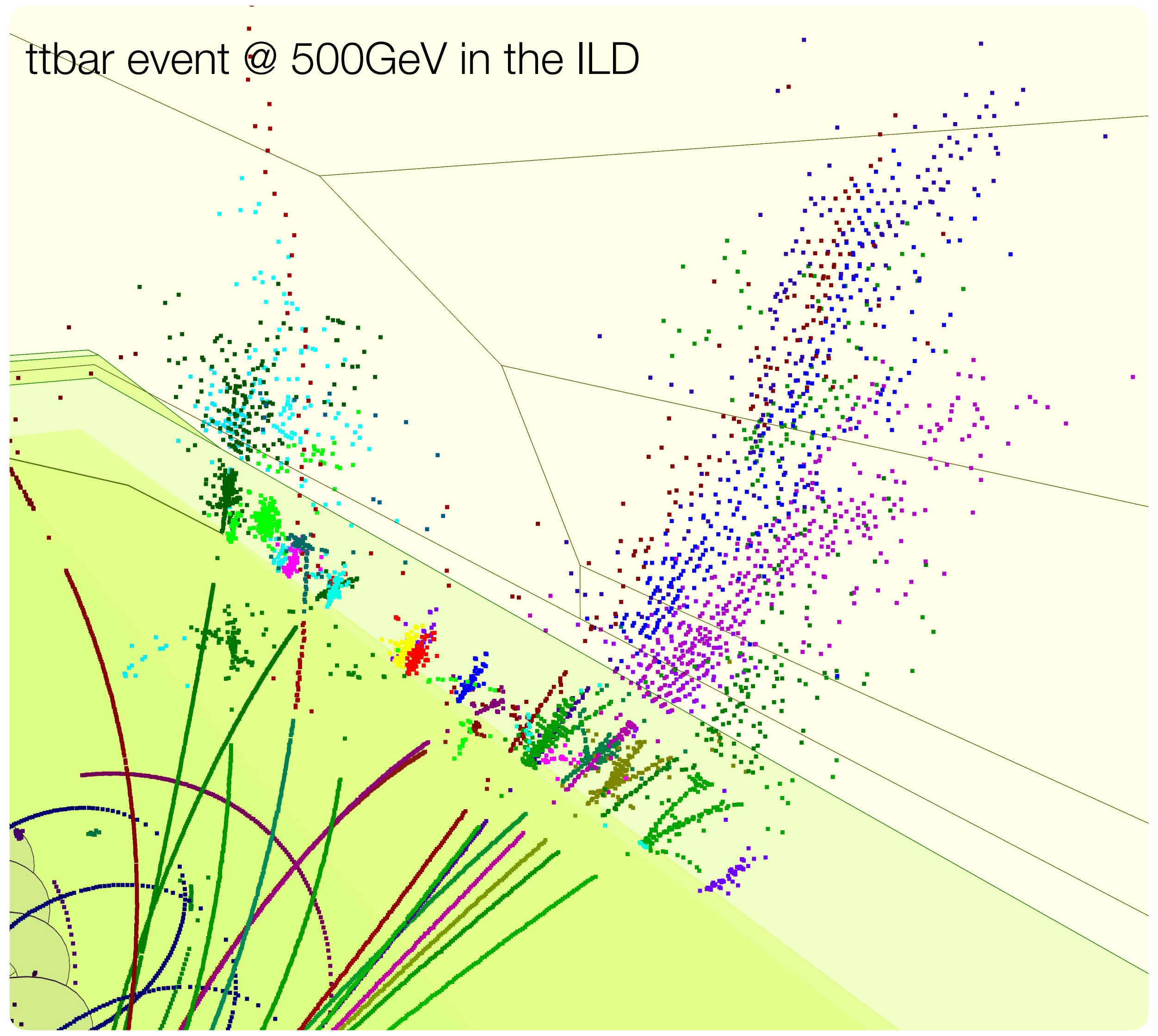
- International Large Detector (ILD) concept for the International Linear Collider (ILC)

- High-Granularity calorimeters:
  - ECal: Si-W - 5mm x 5mm - 30 layers
  - HCal: Sci-Fe - 30mm x 30mm - 48 layers

The International Linear Collider: A Global Project [arxiv: 1903.01629]



High granularity calorimeter ⟶ High fidelity simulation



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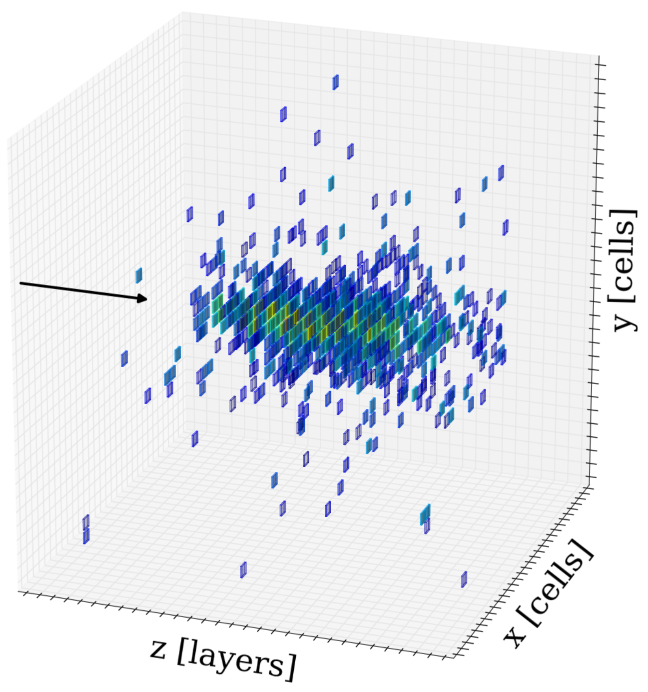
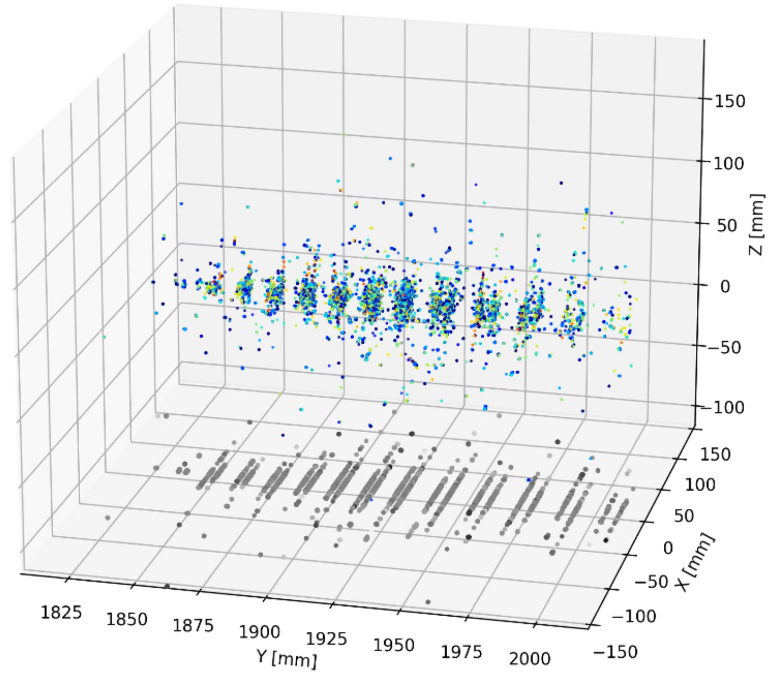
EM shower as 3D image



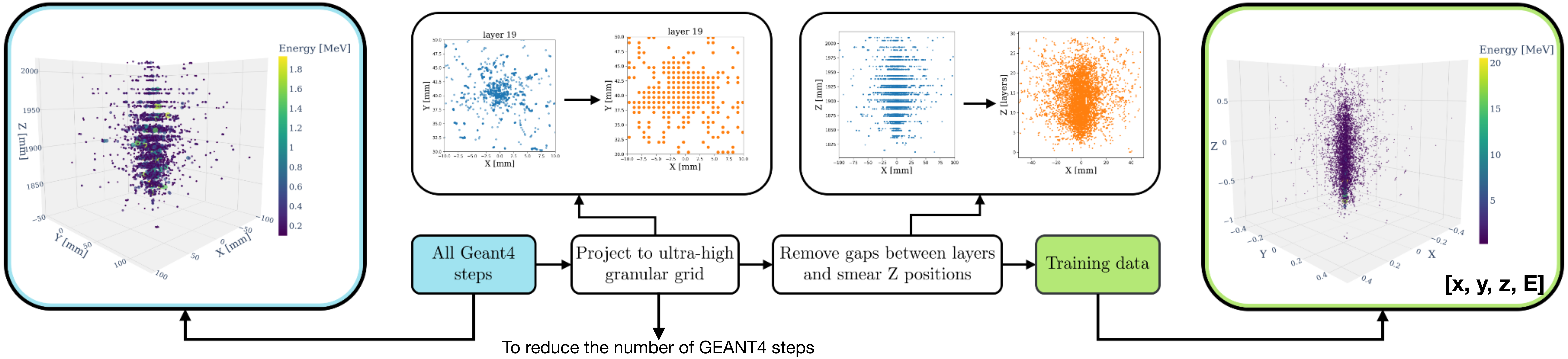
EM shower as point cloud



point clouds

Multiple points per cell & cell-geometry independence

Showers as Point Clouds and Preprocessing



	Photon	Pion+	Note
Shower type	Only em	em + hadronic	
All Geant4 steps	40 000	40 000	Initial input of GEANT4
High granularity	36x	9x	With respect to the calorimeter granularity
High granular cell size	0.3 mm	ECAL: 1.7 mm | HCAL 10 mm	Defines the granularity
Max hits in calorimeter	1 500	**3 000**	Calculation of physics observables

Architecture

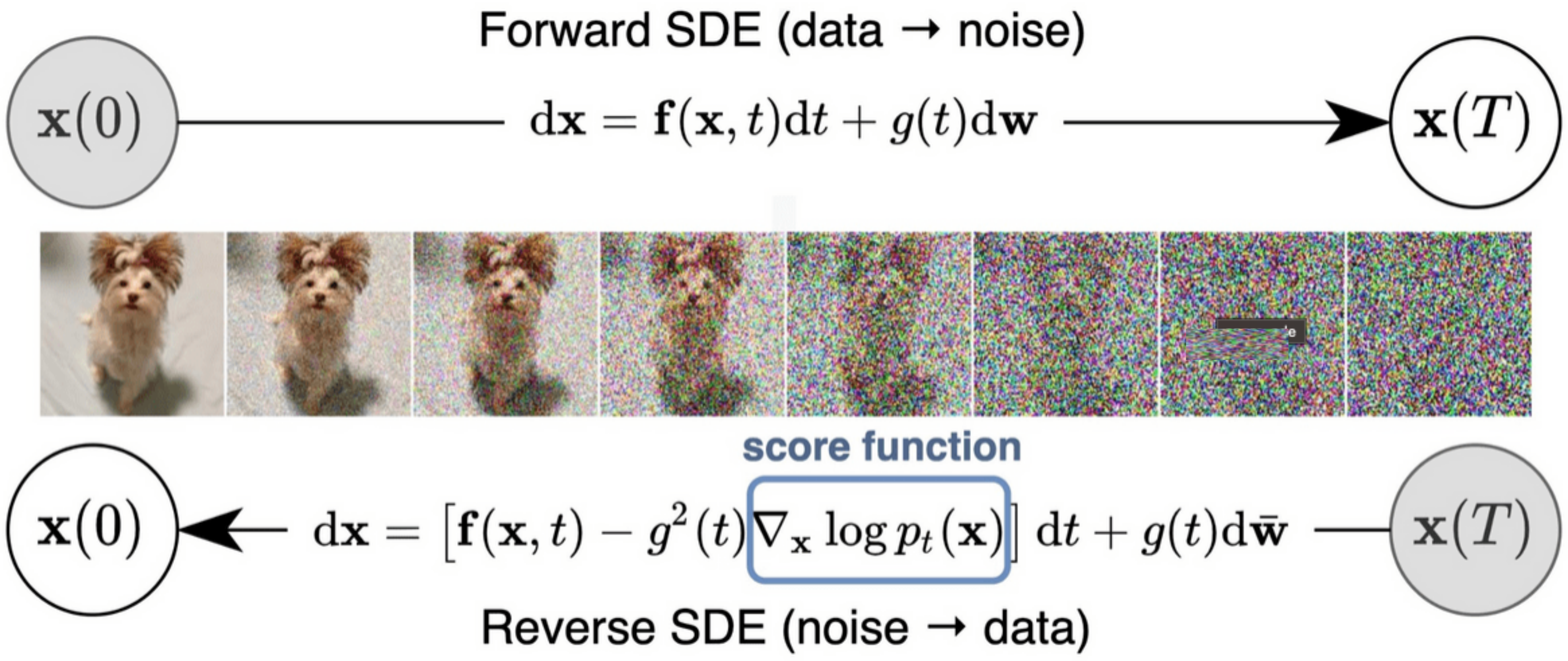
Score-based continuous-time diffusion [2]

Continuous Time:

- this process is modeled by a prescribed stochastic differential equation (SDE)

Score-based:

- score-matching: modelling the gradient of the log probability density function
- langevin dynamics: iterative process that draws samples from a distribution using only its score function



To compute the reverse SDE, we need to estimate the score function:

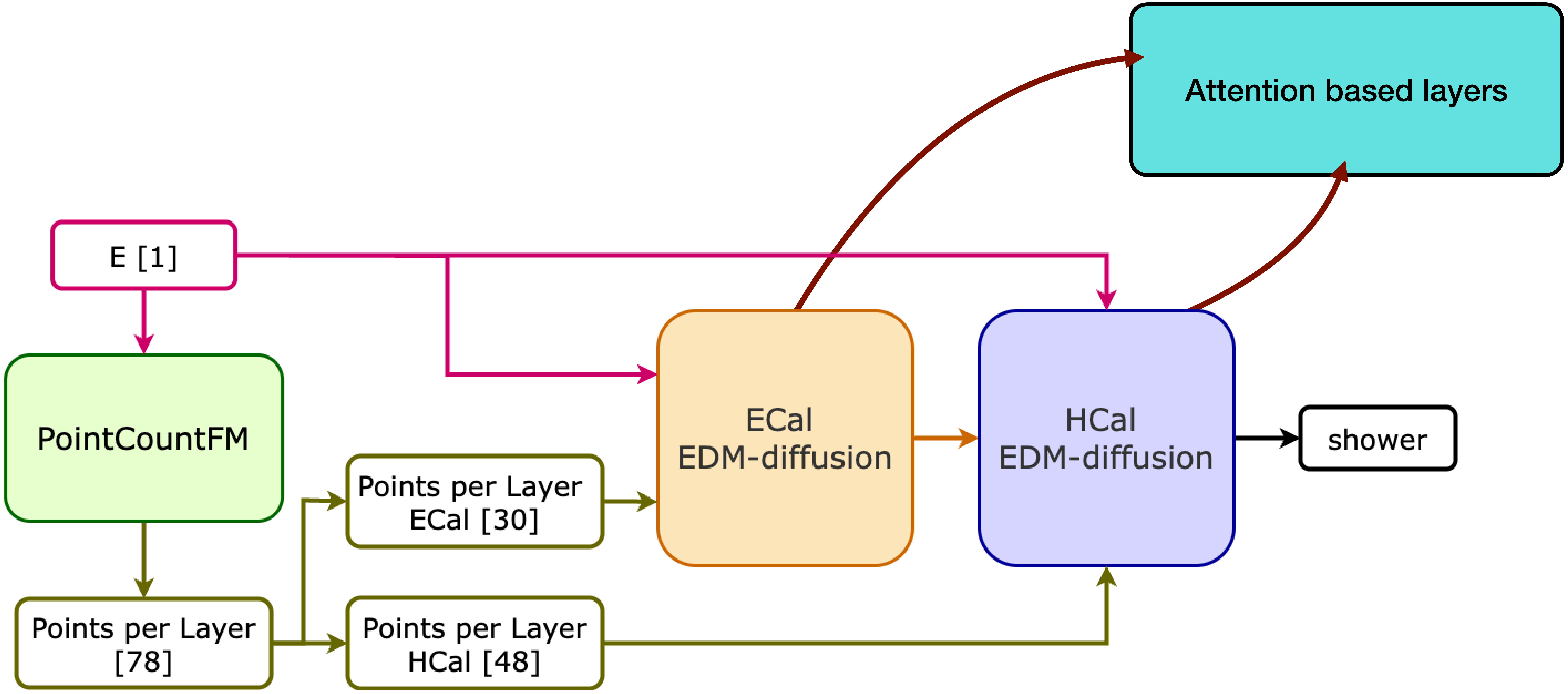
$$\mathbb{E}_{t \in \mathcal{U}(0,T)} \mathbb{E}_{p_t(\mathbf{x})} \left[\lambda(t) \| \nabla_{\mathbf{x}} \log p_t(\mathbf{x}) - \mathbf{s}_\theta(\mathbf{x}, t) \|_2^2 \right]$$

↑ score-based model

[2] Score-based Continuous-time Discrete Diffusion Models
Haoran Sun et al: arxiv: 2211.16750

CaloHadronic

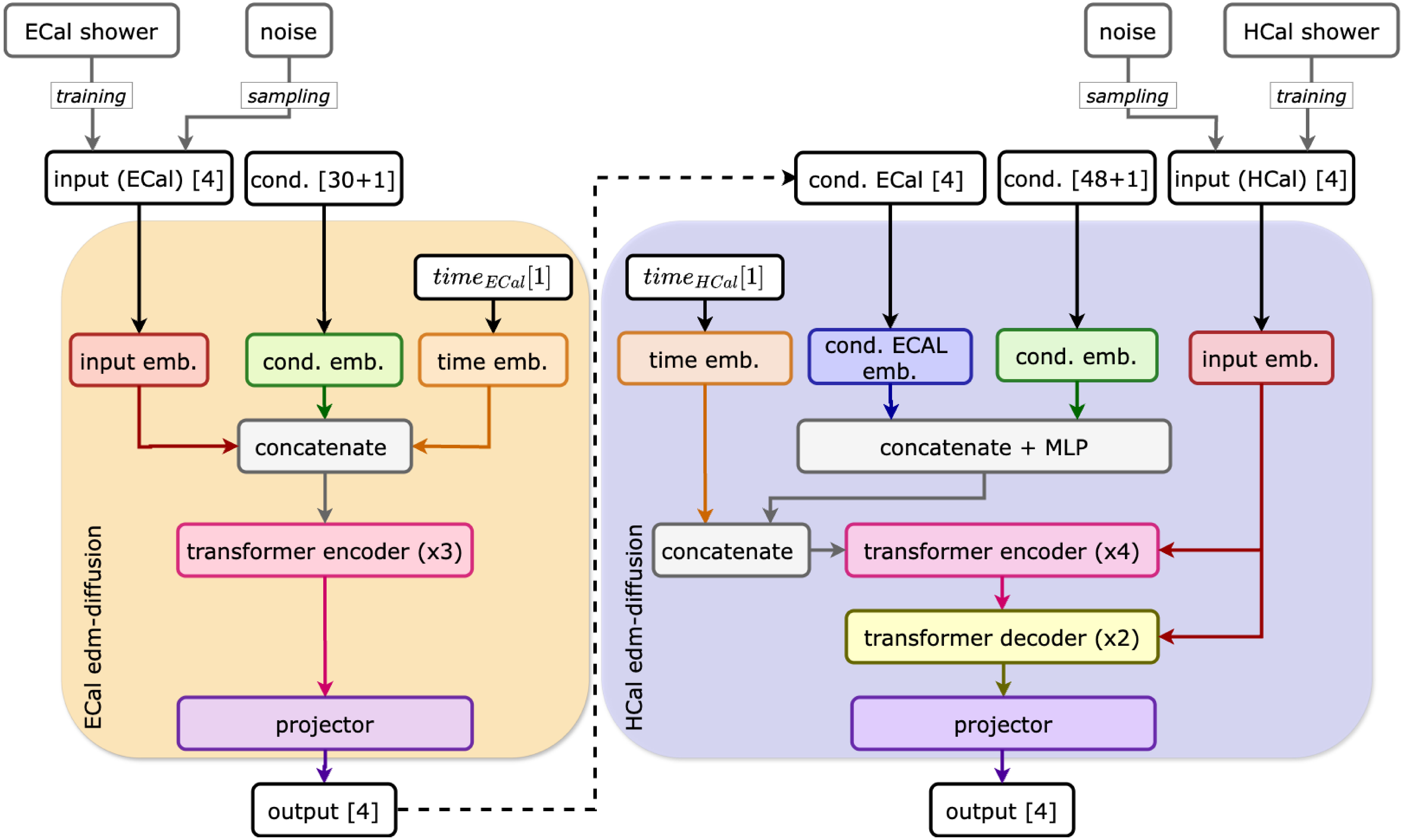
- input: 4D point cloud
- conditioning on: incident energy (E) and number of points per layer
- calibrating on: points per layer



Sampling

CaloHadronic

- input: 4D point cloud
- conditioning on: incident energy (E) and number of points per layer
- calibrating on: points per layer

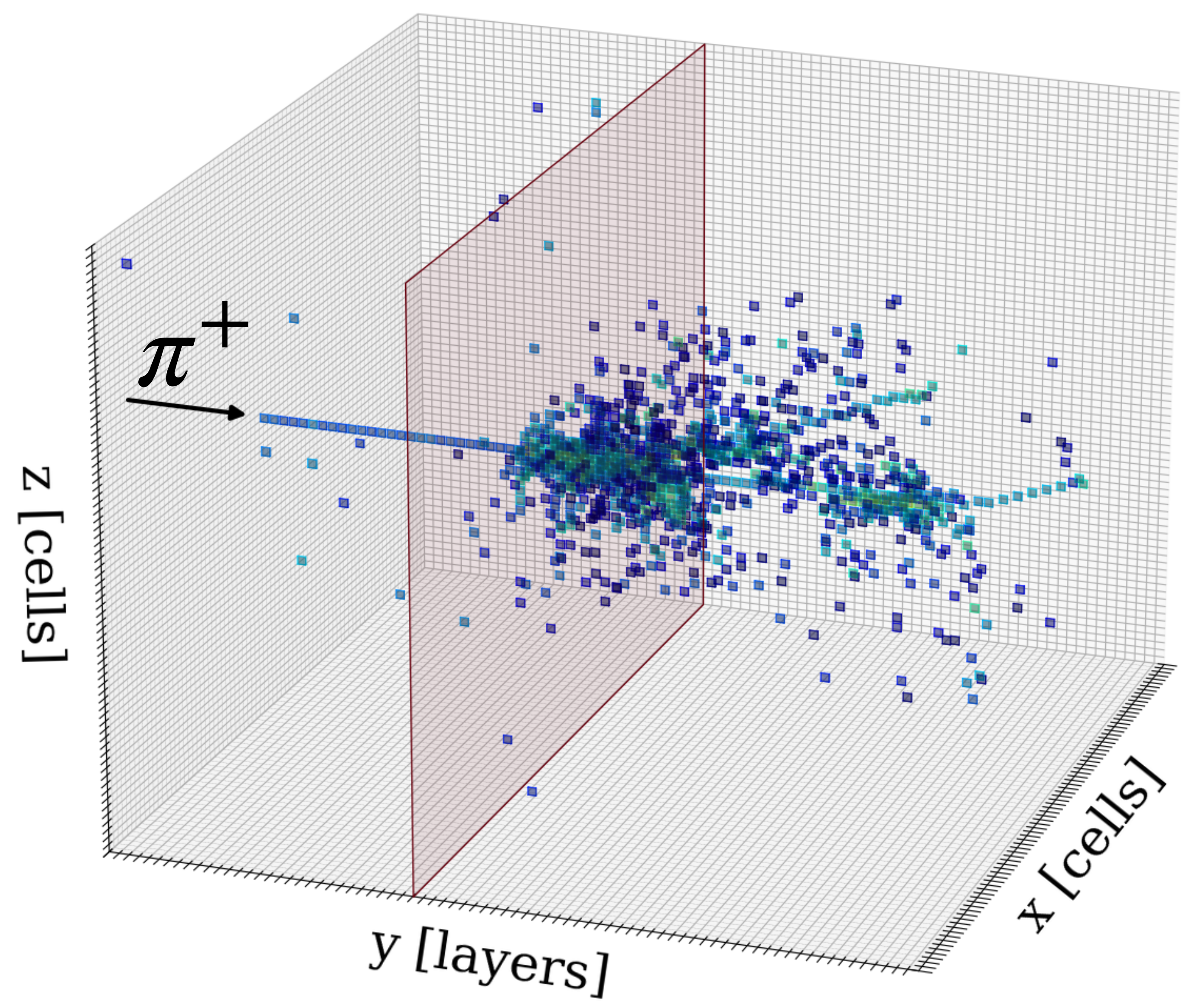


Results

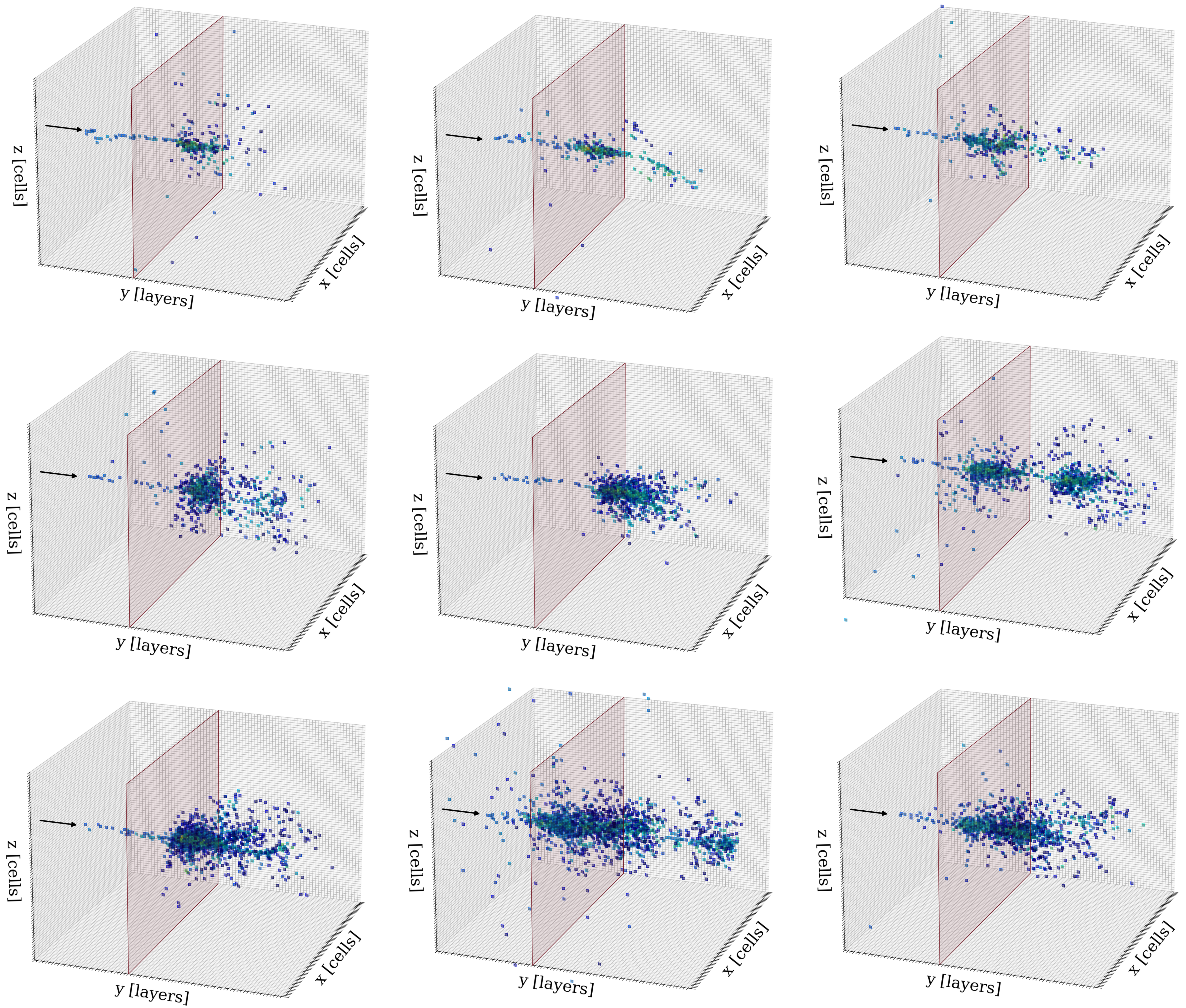
Results

15, 50, 85 GeV π^+ showers

Geant4 Simulation



CaloHadronic



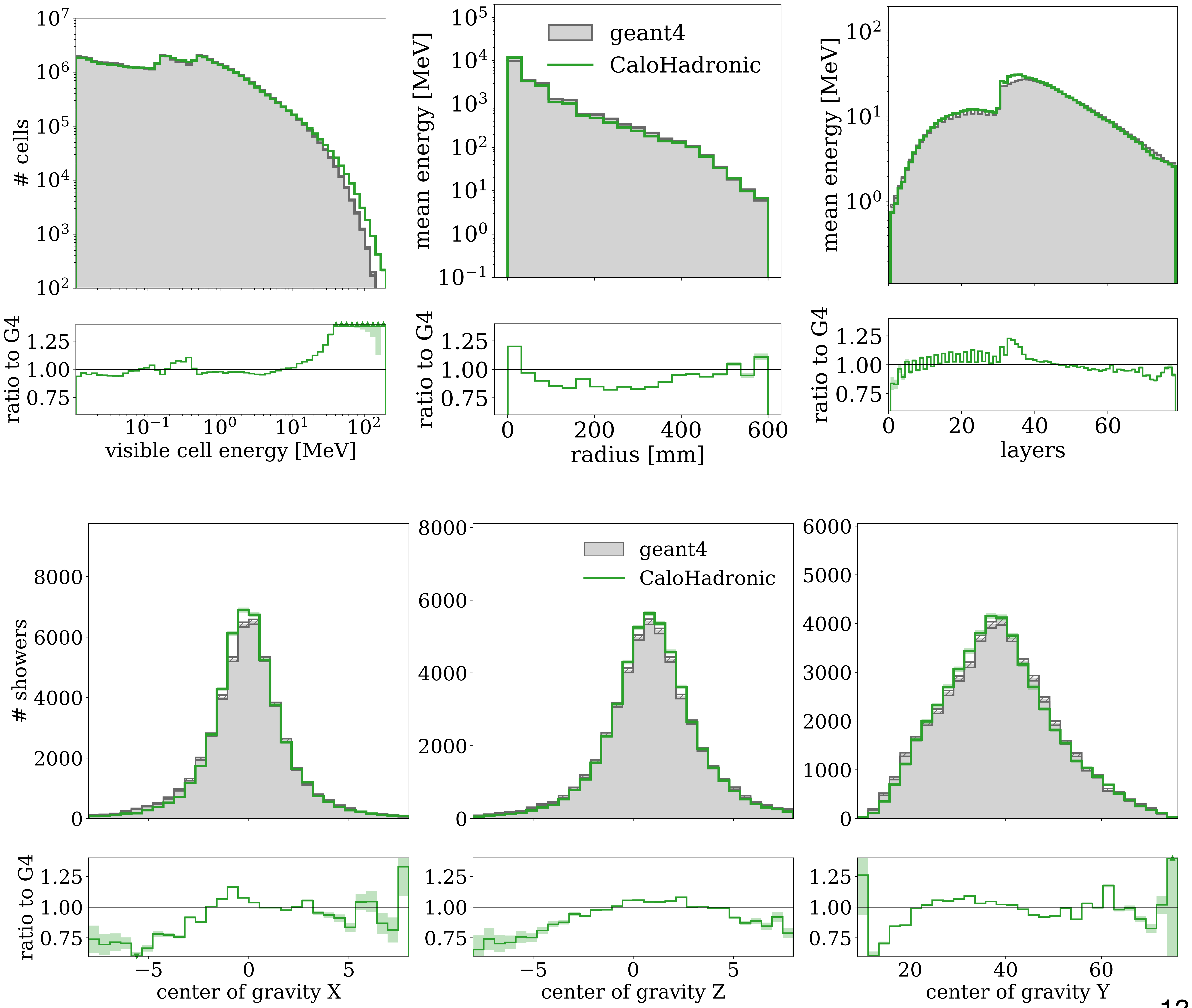
Results

10-90 GeV π⁺ showers

50 000 showers

All evaluations with point cloud showers are projected to a regular cell grid:

ECAL: 5 mm x 30 layers x 5 mm
HCAL: 30 mm x 48 layers x 30 mm



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5 000 showers each

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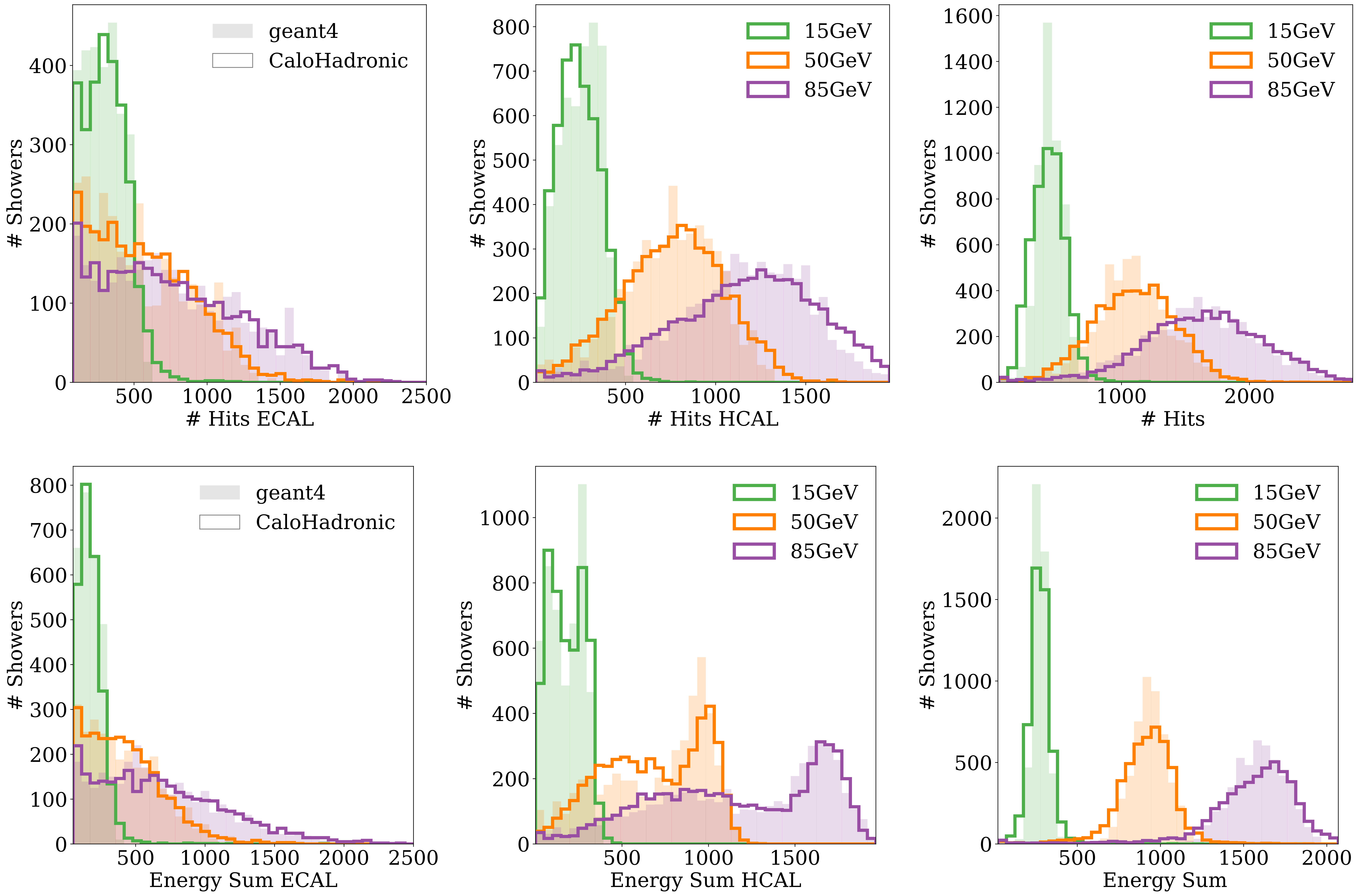
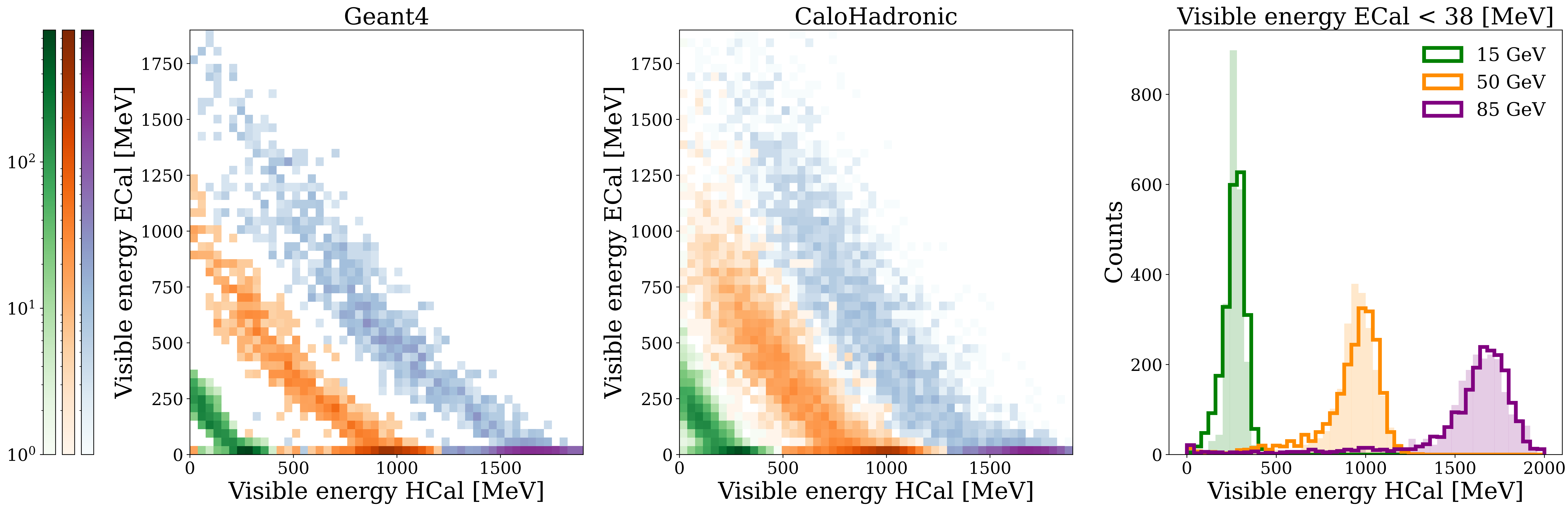


What about correlations?

Results

15, 50 and 85 GeV π⁺ showers

5 000 showers each



Fast calorimeter shower must ultimately be interfaced with the reconstruction chain

Reconstruction with Pandora Particle Flow

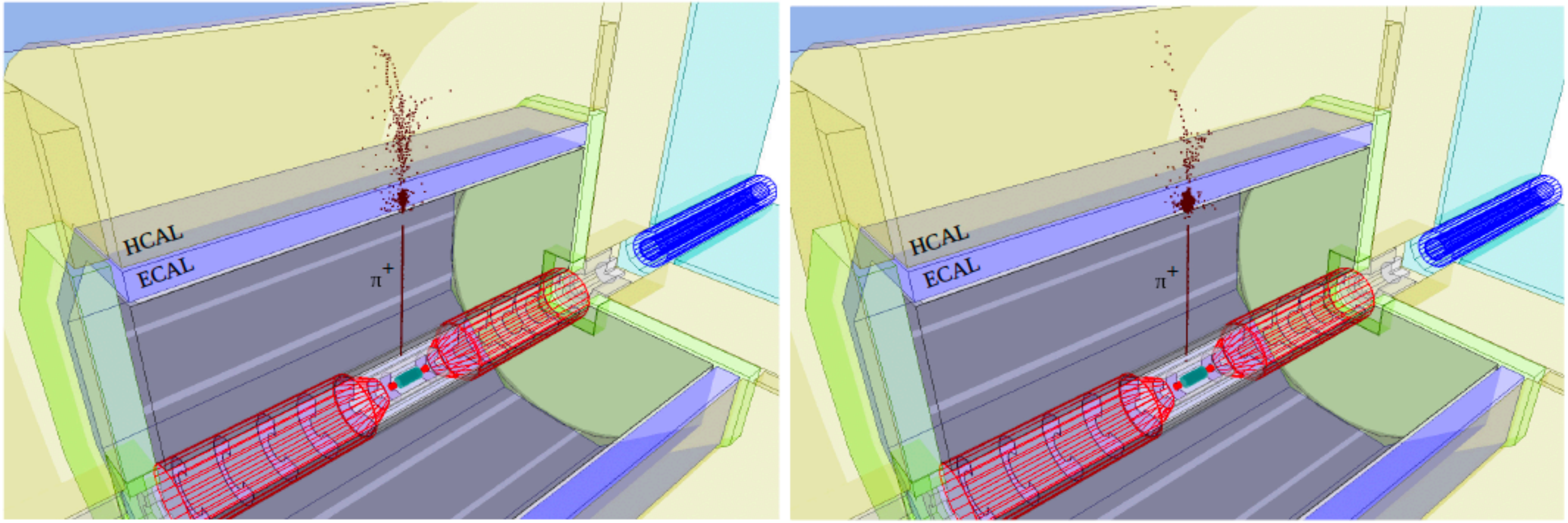


Figure 12. Event displays of Pandora PFOs reconstructed from a Geant4 shower (left), and a CaloHadronic shower (right).

Particle Flow Objects (PFOs): list of reconstructed objects with particle's four-momentum and ID

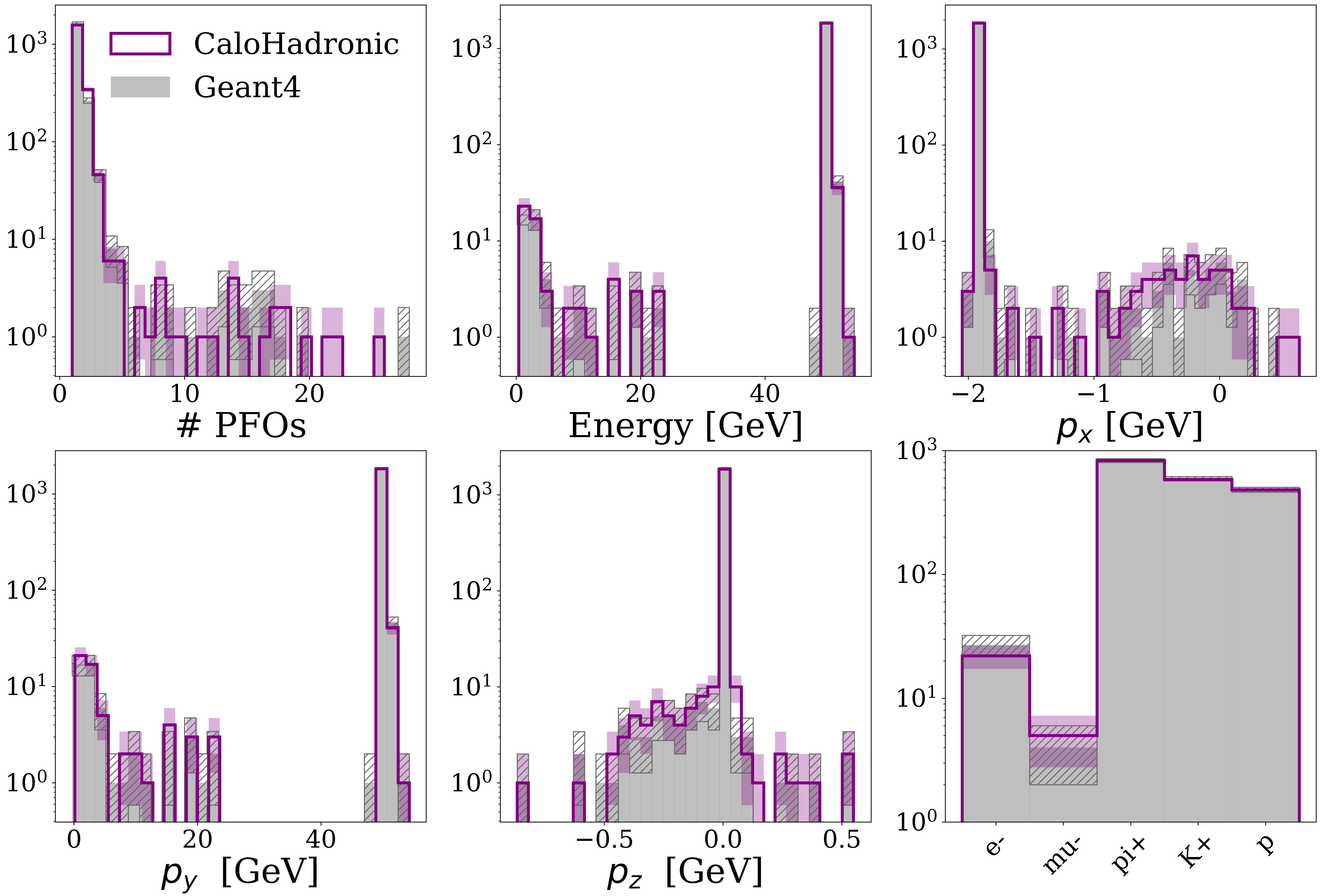
Reconstruction with Pandora Particle Flow

50 GeV π^+ showers

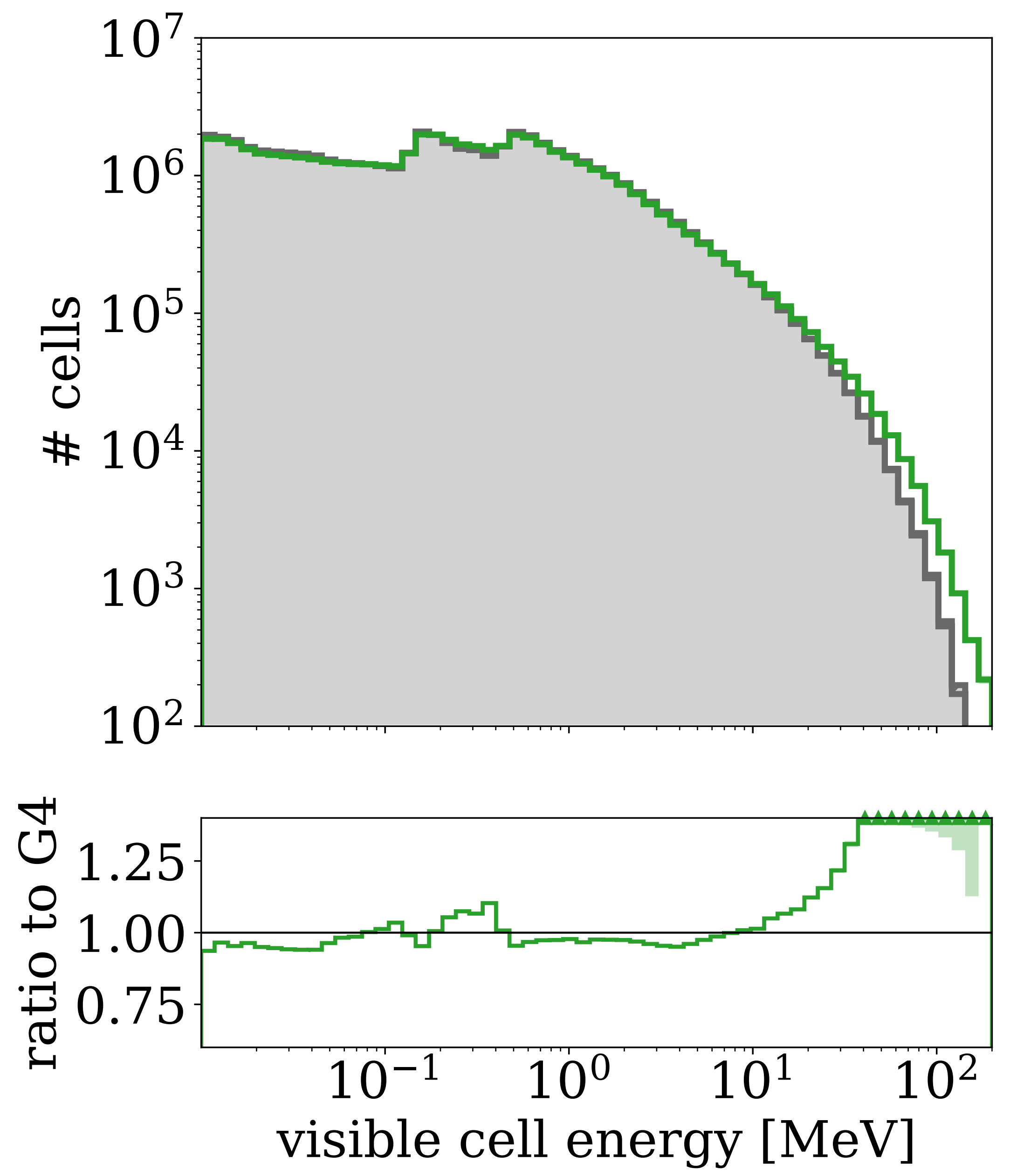
- 2 000 showers

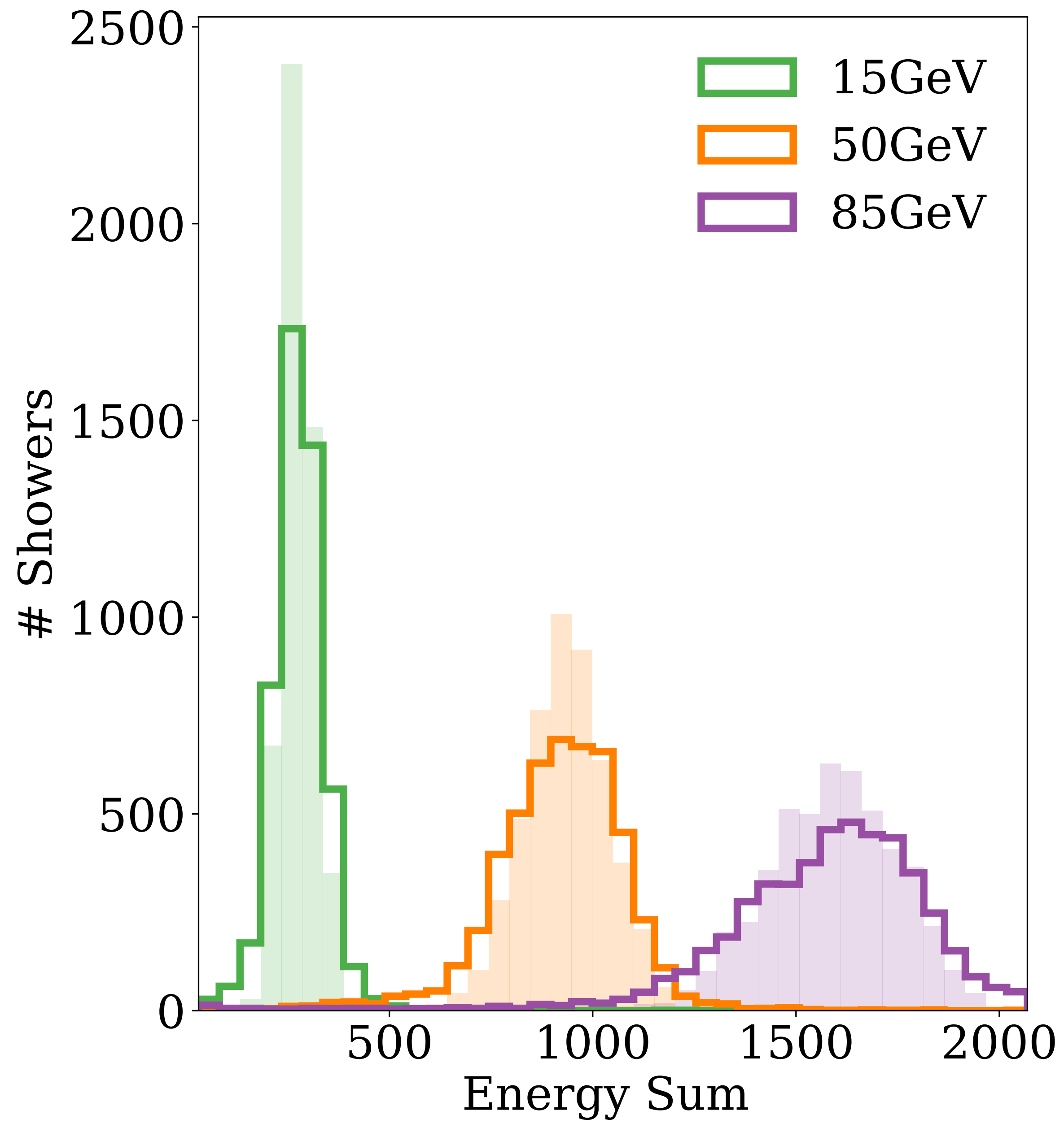
- use the DDML library to combine the model output with a full simulation application

- allows performance validation in realistic detector geometry and in high-level physics observables



Summary





- **First ML based simulation of showers in combined ECAL+HCAL for high granular calorimeters!**
- Clustered Geant4 steps allow for a cell-geometry-independent model
- Attention mechanism is a valid solution —> it considers interactions among points
- Paper out soon —> 2506.XXXXX

Backup

Metrics

10-90 GeV π^+ showers

- 50 000 showers

($\times 10^{-2}$)	cog_x	cog_y	cog_z	Y_{start}	E_{cell}	E_{sum}	E_{radial}	E_{long}	N_{hits}
normalized WD	8.4 ± 0.8	3.8 ± 0.4	8.0 ± 0.7	5.2 ± 0.2	2.8 ± 0.4	9 ± 1	0.05 ± 0.02	76 ± 37	2.8 ± 0.4
quantile KL	1.1 ± 0.3	0.6 ± 0.1	0.9 ± 0.2	2.1 ± 0.2	0.3 ± 0.1	0.68 ± 0.07	0.2 ± 0.2	0.6 ± 0.7	0.3 ± 0.1

Table 4. Wasserstein distances for several physics observables between generated and test data. The Wasserstein distances and the quantile KL are numerically evaluated using five batches of 10,000 showers. Shown are the mean and the standard deviation over the five resulting values.

Simulator	**AUC**	**JSD**
CaloHadronic	0.79 ± 0.03	0.2354 ± 0.0005

Table 5. Results of the high level classifier test. Model performance comparison with area under the receiver operating characteristic curve (AUC) score and Jensen–Shannon divergence (JSD). Shown are the mean and standard deviation over five random network initializations.

Timing

10-90 GeV π^+ showers

- 50 000 showers

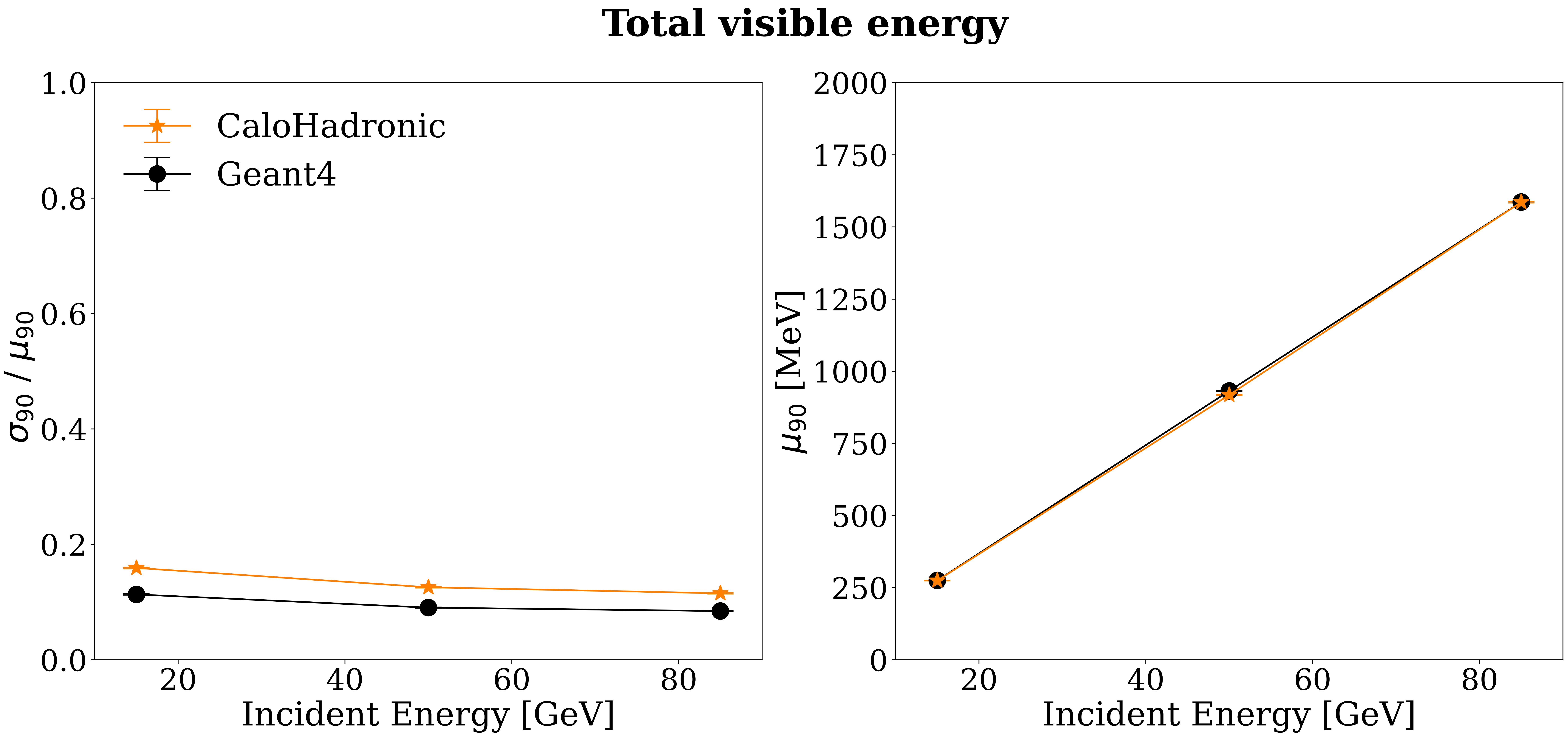
Simulator	Hardware	NFE	Batch Size	Time / Shower [s]	Speed-up
Geant4	CPU		1	2.09 ± 0.05	× 1
CaloHadronic	CPU	1	1	0.591 ± 0.001	× 3.5
			16	0.7342 ± 0.0006	× 2.8
		29	1	17.2 ± 0.1	-
			16	21.37 ± 0.05	-
		59	1	34.8 ± 0.4	-
			16	43.3 ± 0.3	-
	GPU	1	1	0.0086 ± 0.0007	× 243
			16	0.0033 ± 0.0009	× 633
		29	1	0.1978 ± 0.0007	× 11
			16	0.0752 ± 0.0004	× 28
		59	1	0.3962 ± 0.0008	× 5
			16	0.1531 ± 0.0002	× 14

Table 1. Comparison of the computational performance of CaloHadronic to the baseline Geant4 simulator. All CPU runs were performed on a single core of an AMD EPYC 7402 CPU, and GPU runs used an NVIDIA® A100 with 80 GB memory. For each configuration the showers are generated using incident energies ranging from 10 to 90 GeV in 10 GeV increments, with 100 showers per energy point. The mean and standard deviation is computed across three runs. Results show mean ± std over the 3 runs.

Resolution and Linearity

- 5 000 showers each

15, 50 ,85 GeV π^+ showers



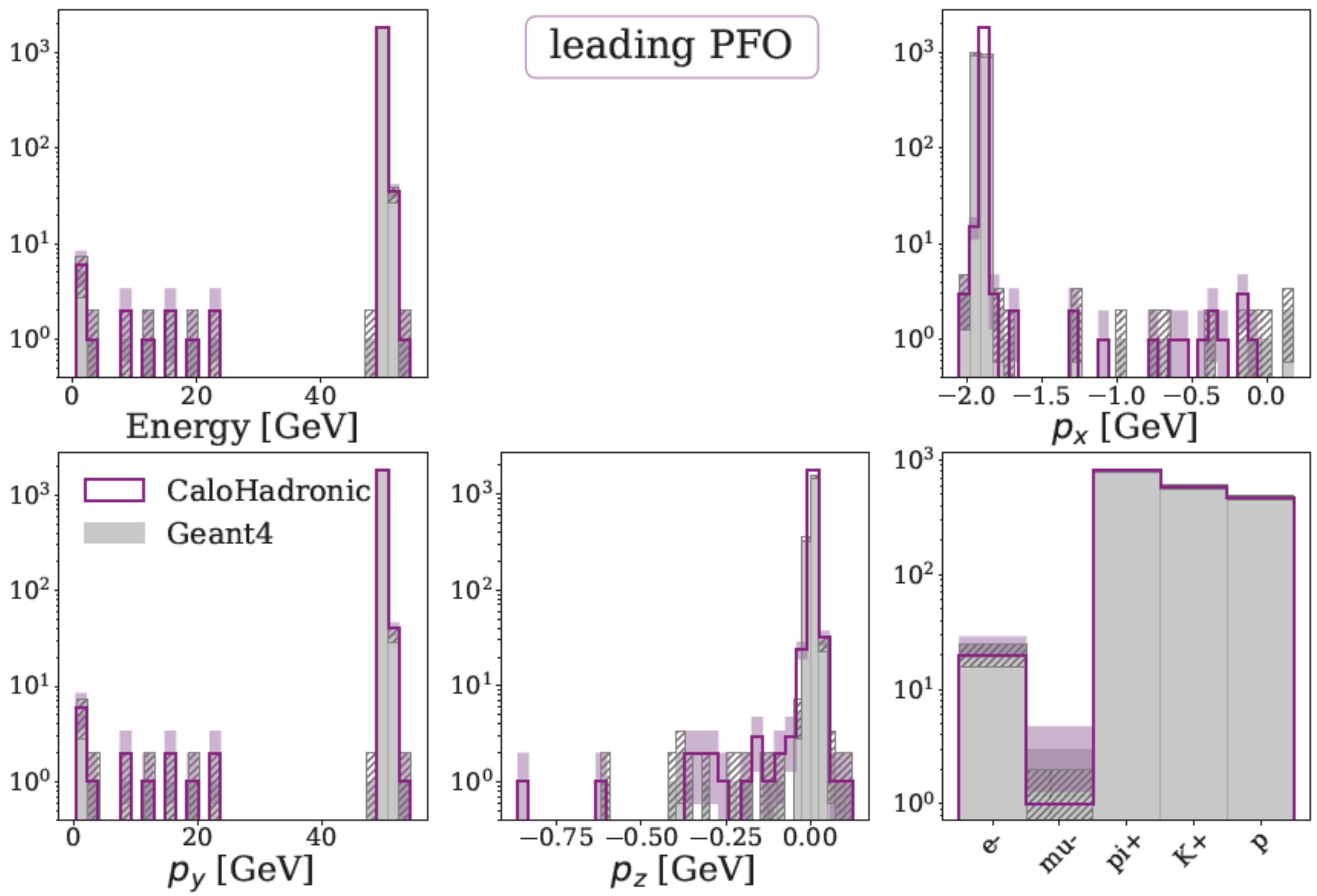


Figure 14. PFO-level observables after reconstruction with PandoraPFA for Geant4 (gray) and CaloHadronic (purple). Only the leading PFO per event is shown. Observables include distributions for the leading PFO energy (top middle), leading PFO momentum in x (p_x, top left), leading PFO momentum in y (p_y, bottom left), leading PFO momentum in z (p_z, bottom middle), and the type of the leading reconstructed particle (bottom right).

Quantitative Measures

- **Normalised Wasserstein Distance:**

$$l_1(P,Q) = \inf_{\pi \in \Gamma(P,Q)} \int_{\mathbb{R}\times\mathbb{R}} |x-y| \, d\pi(x,y)$$

Where $\Gamma(P,Q)$ is the set of (probability) distributions on $\mathbb{R} \times \mathbb{R}$ whose marginals are P and Q on the first and second factors respectively. The final metric is normalised by the standard deviation σ_P of the Geant4 reference.

- **Quantile Kullback-Leibler divergence:**

$$D_{\mathrm{KL}}^{\mathrm{quant}}(P\|Q) = \sum_{i=1}^{N} P_i \log\left(\frac{P_i}{Q_i}\right)$$

  - P_i and Q_i are the probabilities of the Geant4 samples and generated sample falling into the i-th bin, respectively.
  - The bins are defined by the quantiles of the reference sample:

$$\mathrm{bin\_edges} = \left\{-\infty, q_{\frac{0}{N}}, q_{\frac{1}{N}}, \ldots, q_{\frac{N-1}{N}}, +\infty\right\}$$

With q_α being the α-quantile of Geant4 sample.